

# Spurious Shell Closures in the Relativistic Mean Field Model

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Following a systematic theoretical study of the ground-state properties of over 7000 nuclei from the proton drip line to the neutron drip line in the relativistic mean field model [Prog. Theor. Phys. 113 (2005) 785], which is in fair agreement with existing experimental data, we observe a few spurious shell closures, i.e. proton shell closures at  $Z = 58$  and  $Z = 92$ . These spurious shell closures are found to persist in all the effective forces of the relativistic mean field model, e.g. TMA, NL3, PKDD and DD-ME2.

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The relativistic mean field (RMF) model has achieved great successes in studies of nuclear structure for many years.[1, 2, 3] Recently, great efforts in the nuclear physics community have been taken to study exotic nuclei with extreme isospin ratios. In this respect, the RMF model is considered to be a very promising one due to its self-consistent description of the spin-orbit interaction.[4, 5] A careful and systematic study of the ground-state properties of over 7000 nuclei throughout the periodic table has been performed using the RMF+BCS model.[6, 7] It was shown that the RMF model can describe all the ground-state properties of those experimentally known nuclei very well. Nevertheless, a few deficiencies were observed: For example, the neutron skin thickness of  $^{208}\text{Pb}$  is predicted to be 0.26 fm; while recent experimental data seem to be favorable to a smaller value. This deficiency has been (partially) removed by some lately developed effective forces.[8, 9, 10] Another deficiency, which has not received enough attention, is the appearance of spurious shell-closures at  $Z = 58$  and  $Z = 92$ . In Ref. [6], nuclear binding energies around  $^{140}\text{Ce}$  and  $^{218}\text{U}$  were found to be strongly overestimated. A closer examination of the corresponding single-particle spectra showed that they are caused by spurious shell closures at  $Z = 58$  and  $Z = 92$  (just beyond the conventional  $Z = 50$  and  $Z = 82$  shell closures), which are further amplified by the co-occurrence of the  $N = 82$  and  $N = 126$  neutron shell closures.

In this letter, we investigate whether the same spurious shell closures exist in other representative effective forces of the RMF model except TMA [6]. To save space, the formulation of the RMF model is not presented here, which can be easily found in many review articles (see, for example, Ref. [4]). The effective forces we examine in this work are TMA,[11] which has been demonstrated to work very well throughout the periodic table,[6, 7] NL3,[12] one of most-studied effective forces, PKDD,[9] and DD-ME2,[10] two lately developed density-dependent effective forces which have made some improvements compared to older ones. We believe that these four effective forces can represent most existing forces in the current RMF framework. Since an extensive study such as that performed in Ref. [6] is not possible for

all the four forces, we would like to concentrate on  $^{140}\text{Ce}$  and  $^{218}\text{U}$ , where the spurious shell closures at  $Z = 58$  and  $92$  were first clearly identified (see Fig. 2 of Ref. [6]). For comparison, we also study  $^{132}\text{Sn}$  and  $^{208}\text{Pb}$ , which are used as reference nuclei. To avoid any possible ambiguity, all the results shown in this study are obtained with a spherical code and without the pairing correlation. This first approximation is due to the fact that these nuclei are found to be spherical,[6, 13] and the second approximation (together with the first) implies that the so obtained binding energies for these nuclei are at the lower bound.

In Table I, the binding energies of  $^{132}\text{Sn}$ ,  $^{140}\text{Ce}$ ,  $^{208}\text{Pb}$  and  $^{218}\text{U}$  obtained using the effective forces TMA, NL3, PKDD and DD-ME2 are tabulated. It is easily seen that all the four forces overestimate the binding energy of  $^{218}\text{U}$  by at least 8 MeV; while only TMA and PKDD overestimate the binding energy of  $^{140}\text{Ce}$  by the same order. This is in agreement with the systematic study of Ref. [6]. Among the four forces, the latest force DD-ME2 provides the best description of the experimental data, but it still fails for  $^{218}\text{U}$ . This corresponds to the spurious shell closure at  $Z = 92$ , as we shall see in the following. It is interesting to note that PKDD does particularly well for  $^{132}\text{Sn}$  and  $^{208}\text{Pb}$  while it is not so good for  $^{140}\text{Ce}$  and  $^{218}\text{U}$ . Considering that these effective forces describe most nuclei throughout the periodic table with

TABLE I: Binding energies of  $^{132}\text{Sn}$ ,  $^{208}\text{Pb}$ ,  $^{140}\text{Ce}$  and  $^{218}\text{U}$  obtained with effective forces TMA, NL3, PKDD and DD-ME2 (in units of MeV). The experimental data are taken from Ref. [14].

	$^{132}\text{Sn}$	$^{208}\text{Pb}$	$^{140}\text{Ce}$	$^{218}\text{U}$
TMA	1103.4	1634.7	1179.4	1674.0
NL3	1103.2	1637.5	1176.3	1674.7
PK-DD	1102.6	1637.2	1179.0	1677.7
DD-ME2	1103.5	1639.0	1175.9	1673.5
Exp.	1102.9	1636.4	1172.7	1665.6

TABLE II: Proton shell closures at  $Z = 50, 58$  in  $^{132}\text{Sn}$  ( $^{140}\text{Ce}$ ) and those at  $Z = 82, 92$  in  $^{208}\text{Pb}$  ( $^{218}\text{U}$ ) obtained with effective forces TMA, NL3, PKDD and DD-ME2 (in units of MeV). The first column under  $^{132}\text{Sn}$  ( $^{140}\text{Ce}$ ) is the shell closure at  $Z = 50$  and the second column is that at  $Z = 58$ . The first column under  $^{208}\text{Pb}$  ( $^{218}\text{U}$ ) is the shell closure at  $Z = 82$  while the second column is that at  $Z = 92$ .

	$^{132}\text{Sn}$		$^{140}\text{Ce}$		$^{208}\text{Pb}$		$^{218}\text{U}$	
TMA	5.66	3.73	5.36	4.12	2.47	4.01	2.34	3.93
NL3	6.15	2.81	5.78	3.50	3.50	3.20	3.14	3.54
PKDD	6.45	2.99	6.09	3.63	3.59	3.36	3.25	3.63
DD-ME2	6.45	2.39	6.01	3.08	4.06	2.74	3.64	3.28
Exp.	6.03	0.96			4.20	0.90		

a discrepancy of 2–3 MeV,[6, 13] the 8 MeV discrepancy is rather large. This therefore indicates some physics that should not be ignored. Following Bertsch *et al.*[15] these nuclei should be thought of as “critical nuclei” of the corresponding forces.

In Ref. [6], the overbindings of  $^{140}\text{Ce}$  and  $^{218}\text{U}$  were attributed to the corresponding spurious shell closures at  $Z = 58$  and  $Z = 92$ . In the following, we investigate whether it is still the case for NL3, PKDD and DD-ME2. The proton shell closures at  $Z = 50, 58$  in  $^{132}\text{Sn}$  ( $^{140}\text{Ce}$ ) and those at  $Z = 82, 92$  in  $^{208}\text{Pb}$  ( $^{218}\text{U}$ ) obtained with effective forces TMA, NL3, PKDD and DD-ME2 are tabulated in Table II. For comparison, the experimental data for  $^{132}\text{Sn}$  and  $^{208}\text{Pb}$  are also shown. For  $^{132}\text{Sn}$ , it is seen that NL3 agrees with experiment best; TMA underestimates the  $Z = 50$  shell closure but overestimates the  $Z = 58$  shell closure; while PKDD and DD-ME2 are of similar quality. The large  $Z = 58$  shell closure in TMA and PKDD persists even at  $^{140}\text{Ce}$ , which explains the overbinding of this nucleus as listed in Table I. For  $^{208}\text{Pb}$ , DD-ME2 agrees with experiment best; TMA underestimates the  $Z = 82$  shell closure but overestimates the  $Z = 92$  shell closure; while NL3 and PKDD are of similar quality. For  $^{218}\text{U}$ , all the effective forces predict a very large shell closure at  $Z = 92$ : it is even larger than that at 82 in TMA, NL3 and PKDD; while in DD-ME2 it is slightly smaller than that at 82. This extremely large  $Z = 92$  shell closure is believed to be responsible for the overbinding of  $^{218}\text{U}$  as listed in Table I. It is interesting to note that the existence of these spurious shell closures seems to be a common feature of the current RMF forces (at least for those investigated here), while in nonrelativistic Hartree-Fock models, no such a common feature has been found.

The nucleus is composed of both protons and neutrons. Therefore, one must study not only protons but also neutrons to obtain a complete picture. In Table III, the neutron shell closures at  $N = 82$  in  $^{132}\text{Sn}$  ( $^{140}\text{Ce}$ ) and those at  $N = 126$  in  $^{208}\text{Pb}$  ( $^{218}\text{U}$ ) obtained with effective forces TMA, NL3, PKDD and DD-ME2 are tabulated. It is seen that all the effective forces overestimate the  $N = 82$  shell closure by about 1.5 MeV. From  $^{132}\text{Sn}$  to  $^{140}\text{Ce}$ , this shell closure increases in NL3, PKDD and DD-ME2;

TABLE III: Neutron shell closures at  $N = 82$  in  $^{132}\text{Sn}$  ( $^{140}\text{Ce}$ ) and those at  $N = 126$  in  $^{208}\text{Pb}$  ( $^{218}\text{U}$ ) obtained with effective forces TMA, NL3, PKDD and DD-ME2 (in units of MeV).

	$^{132}\text{Sn}$	$^{140}\text{Ce}$	$^{208}\text{Pb}$	$^{218}\text{U}$
TMA	6.78	5.58	3.58	2.14
NL3	6.17	6.38	4.60	3.07
PKDD	6.50	6.65	4.78	3.16
DD-ME2	6.17	7.07	5.25	3.72
Exp.	4.84		3.43	

while it decreases in TMA. For  $^{208}\text{Pb}$ , TMA agrees with experiment very well; while all the others overestimate the experimental value with DD-ME2 having the largest discrepancy. From  $^{208}\text{Pb}$  to  $^{218}\text{U}$ , a decrease of about 1.5 MeV is seen for all the effective forces. From Table II and Table III, it can be concluded that the better description of the proton shell closure of  $^{208}\text{Pb}$  in NL3, PKDD and DD-ME2 compared to TMA is at the expense of the overestimation of the neutron shell closure, which is particularly true for DD-ME2.

The importance of identifying these spurious shell closures or “critical nuclei” can be summarized as follows: (i) It points out the regions in the periodic table that the present RMF model can not describe so well. (ii) It tells us to further study what causes these spurious shell closures and how to remove them. As a result, the current formulation of the RMF model can be improved. In the following, we discuss several approaches that might be helpful to remove the observed spurious shell closures. It should be noted that our discussions are restricted to the mean-field level and are not meant to be exhaustive. First, one may need a more balanced fitting strategy. For example, only the ground-state properties of twelve nuclei are fitted to obtain the latest effective force DD-ME2. Meanwhile these twelve nuclei are in some sense neutron rich. Since all the current effective forces in the RMF model adopt a similar procedure to fix their parameter values, it is unsurprising that they all overestimate  $^{218}\text{U}$ , which is proton rich. Although an extensive fitting

TABLE IV: Binding energies of  $^{132}\text{Sn}$ ,  $^{208}\text{Pb}$ ,  $^{140}\text{Ce}$  and  $^{218}\text{U}$  obtained with effective forces DD-ME2 and DD-ME2(M) (in units of MeV). The experimental data are taken from Ref. [14].

	$^{132}\text{Sn}$	$^{208}\text{Pb}$	$^{140}\text{Ce}$	$^{218}\text{U}$
DD-ME2	1103.5	1639.0	1175.9	1673.5
DD-ME2(M)	1100.6	1634.4	1172.9	1168.7
Exp.	1102.9	1636.4	1172.7	1665.6

strategy such as that used in obtaining the latest series of Hartree-Fock-Bogoliubov mass tables [16] in the RMF model is not likely to be carried out in the near future, a more balanced fitting strategy can hopefully remove or at least reduce the overbinding of  $^{218}\text{U}$  and those around it. In this sense, taking into account the single-particle spectra, in particular those of  $^{208}\text{Pb}$ , during the fitting process might also improve the description of these critical nuclei.

Another alternative is to make magic nuclei slightly less bound. The reason is that particle-number conserved pairing methods usually give a few MeV of energy gain to even magic nuclei.[17] Therefore, fitting the binding energies of magic nuclei exactly to the experimental data or even slightly larger than the experimental data (most current RMF forces behave in this way) leaves no room for further improvement and meanwhile overestimates magic number effects. Just to see how we can reduce the overbindings of  $^{140}\text{Ce}$  and  $^{218}\text{U}$  by making magic nu-

clei, particularly  $^{132}\text{Sn}$  and  $^{208}\text{Pb}$ , less bound, we modify the effective force DD-ME2. It should be noted that the purpose is not to develop a new effective force, but to demonstrate our above statements. To keep things simple, we only change the nucleon masses. The nucleon masses used in DD-ME2 are 939.0 MeV for both protons and neutrons.[18] We reduce them to 938.5 MeV. The binding energies obtained with this modified DD-ME2 (denoted as DD-ME2(M)) for  $^{132}\text{Sn}$ ,  $^{140}\text{Ce}$ ,  $^{208}\text{Pb}$  and  $^{218}\text{U}$  are tabulated in Table IV. One can easily see that now the discrepancies are more evenly distributed, i.e. serious discrepancies disappear.

To make RMF calculations more reliable for astrophysical studies and/or studies of exotic nuclei, the predictions of nuclear masses must be improved. It may or may not be possible within the current formulation of the RMF model. One may finally resort to a similar procedure adopted in non-relativistic calculations.[16] Although recently constructed effective forces do show improvements compared to older ones, deficiencies remain as demonstrated in this work. The recent systematic study [6] showed that most discrepancies between the RMF results and existing experimental data actually originate from the regions surrounding the so-called critical nuclei. Therefore, removing them should be viewed as an essential criteria for the next-generation effective forces. These works are underway.

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